

Triethylenetetramine
112-24-3 | DTXSID9023702

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 29.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.54e-01

Confidence level: 5.17e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cymoxanil</div> <div>Measured: 123</div> <div>Predicted: 72.0</div>	<div>Image not found</div> <div>Diethanolamine</div> <div>Measured: 3.98</div> <div>Predicted: 4.00</div>	<div>Image not found</div> <div>Glufosinate-ammonium</div> <div>Measured: 427</div> <div>Predicted: 194</div>
<div>Image not found</div> <div>1-Methoxy-2-propyl acetate</div> <div>Measured: 2.29</div> <div>Predicted: 7.33</div>	<div>Image not found</div> <div>2-(Pyridin-2-yl)ethanol</div> <div>Measured: 28.2</div> <div>Predicted: 35.9</div>	